



# wwPDB X-ray Structure Validation Summary Report

Jan 20, 2024 – 02:06 pm GMT

PDB ID : 7AZL  
Title : DNA polymerase sliding clamp from Escherichia coli with peptide 38 bound  
Authors : Monsarrat, C.; Compain, G.; Andre, C.; Martiel, I.; Engilberge, S.; Olieric, V.; Wolff, P.; Brillet, K.; Landolfo, M.; Silva da Veiga, C.; Wagner, J.; Guichard, G.; Burnouf, D.Y.  
Deposited on : 2020-11-16  
Resolution : 2.42 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

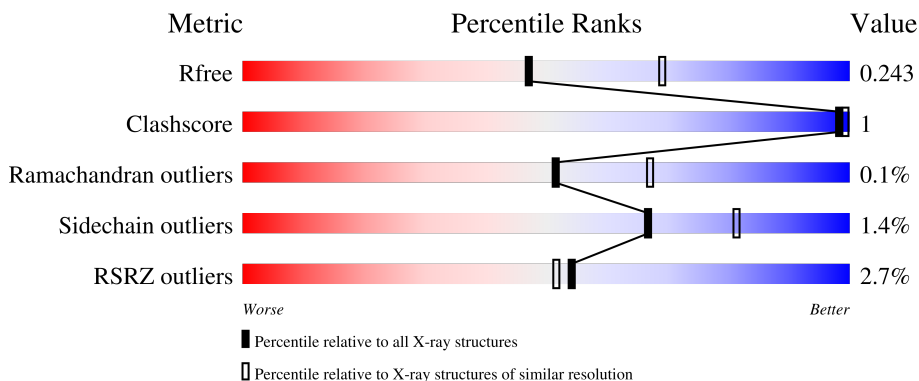
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




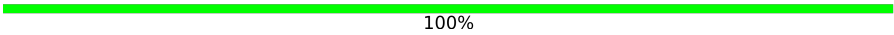

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	 90% 6%
1	B	386	 4% 91% 7%
1	C	386	 2% 91% 6%
1	D	386	 3% 90% 7%
2	E	6	 83% 17%

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Mol	Chain	Length	Quality of chain
2	F	6	 83% 17%
2	G	6	 100%
2	H	6	 100%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11848 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2808	1762	487	540	19	0	1	0
1	B	358	2778	1747	484	528	19	0	0	0
1	C	361	2798	1762	487	530	19	0	2	0
1	D	359	2773	1750	482	522	19	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A073FMV0
A	-18	GLY	-	expression tag	UNP A0A073FMV0
A	-17	SER	-	expression tag	UNP A0A073FMV0
A	-16	SER	-	expression tag	UNP A0A073FMV0
A	-15	HIS	-	expression tag	UNP A0A073FMV0
A	-14	HIS	-	expression tag	UNP A0A073FMV0
A	-13	HIS	-	expression tag	UNP A0A073FMV0
A	-12	HIS	-	expression tag	UNP A0A073FMV0
A	-11	HIS	-	expression tag	UNP A0A073FMV0
A	-10	HIS	-	expression tag	UNP A0A073FMV0
A	-9	SER	-	expression tag	UNP A0A073FMV0
A	-8	SER	-	expression tag	UNP A0A073FMV0
A	-7	GLY	-	expression tag	UNP A0A073FMV0
A	-6	LEU	-	expression tag	UNP A0A073FMV0
A	-5	VAL	-	expression tag	UNP A0A073FMV0
A	-4	PRO	-	expression tag	UNP A0A073FMV0
A	-3	ARG	-	expression tag	UNP A0A073FMV0
A	-2	GLY	-	expression tag	UNP A0A073FMV0
A	-1	SER	-	expression tag	UNP A0A073FMV0
A	0	HIS	-	expression tag	UNP A0A073FMV0
B	-19	MET	-	initiating methionine	UNP A0A073FMV0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A073FMV0
B	-17	SER	-	expression tag	UNP A0A073FMV0
B	-16	SER	-	expression tag	UNP A0A073FMV0
B	-15	HIS	-	expression tag	UNP A0A073FMV0
B	-14	HIS	-	expression tag	UNP A0A073FMV0
B	-13	HIS	-	expression tag	UNP A0A073FMV0
B	-12	HIS	-	expression tag	UNP A0A073FMV0
B	-11	HIS	-	expression tag	UNP A0A073FMV0
B	-10	HIS	-	expression tag	UNP A0A073FMV0
B	-9	SER	-	expression tag	UNP A0A073FMV0
B	-8	SER	-	expression tag	UNP A0A073FMV0
B	-7	GLY	-	expression tag	UNP A0A073FMV0
B	-6	LEU	-	expression tag	UNP A0A073FMV0
B	-5	VAL	-	expression tag	UNP A0A073FMV0
B	-4	PRO	-	expression tag	UNP A0A073FMV0
B	-3	ARG	-	expression tag	UNP A0A073FMV0
B	-2	GLY	-	expression tag	UNP A0A073FMV0
B	-1	SER	-	expression tag	UNP A0A073FMV0
B	0	HIS	-	expression tag	UNP A0A073FMV0
C	-19	MET	-	initiating methionine	UNP A0A073FMV0
C	-18	GLY	-	expression tag	UNP A0A073FMV0
C	-17	SER	-	expression tag	UNP A0A073FMV0
C	-16	SER	-	expression tag	UNP A0A073FMV0
C	-15	HIS	-	expression tag	UNP A0A073FMV0
C	-14	HIS	-	expression tag	UNP A0A073FMV0
C	-13	HIS	-	expression tag	UNP A0A073FMV0
C	-12	HIS	-	expression tag	UNP A0A073FMV0
C	-11	HIS	-	expression tag	UNP A0A073FMV0
C	-10	HIS	-	expression tag	UNP A0A073FMV0
C	-9	SER	-	expression tag	UNP A0A073FMV0
C	-8	SER	-	expression tag	UNP A0A073FMV0
C	-7	GLY	-	expression tag	UNP A0A073FMV0
C	-6	LEU	-	expression tag	UNP A0A073FMV0
C	-5	VAL	-	expression tag	UNP A0A073FMV0
C	-4	PRO	-	expression tag	UNP A0A073FMV0
C	-3	ARG	-	expression tag	UNP A0A073FMV0
C	-2	GLY	-	expression tag	UNP A0A073FMV0
C	-1	SER	-	expression tag	UNP A0A073FMV0
C	0	HIS	-	expression tag	UNP A0A073FMV0
D	-19	MET	-	initiating methionine	UNP A0A073FMV0
D	-18	GLY	-	expression tag	UNP A0A073FMV0
D	-17	SER	-	expression tag	UNP A0A073FMV0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A073FMV0
D	-15	HIS	-	expression tag	UNP A0A073FMV0
D	-14	HIS	-	expression tag	UNP A0A073FMV0
D	-13	HIS	-	expression tag	UNP A0A073FMV0
D	-12	HIS	-	expression tag	UNP A0A073FMV0
D	-11	HIS	-	expression tag	UNP A0A073FMV0
D	-10	HIS	-	expression tag	UNP A0A073FMV0
D	-9	SER	-	expression tag	UNP A0A073FMV0
D	-8	SER	-	expression tag	UNP A0A073FMV0
D	-7	GLY	-	expression tag	UNP A0A073FMV0
D	-6	LEU	-	expression tag	UNP A0A073FMV0
D	-5	VAL	-	expression tag	UNP A0A073FMV0
D	-4	PRO	-	expression tag	UNP A0A073FMV0
D	-3	ARG	-	expression tag	UNP A0A073FMV0
D	-2	GLY	-	expression tag	UNP A0A073FMV0
D	-1	SER	-	expression tag	UNP A0A073FMV0
D	0	HIS	-	expression tag	UNP A0A073FMV0

- Molecule 2 is a protein called Peptide 38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	E	6	Total	C	Cl	N	O	0	0	0
			61	42	2	7	10			
2	G	6	Total	C	Cl	N	O	0	1	0
			70	47	2	8	13			
2	F	6	Total	C	Cl	N	O	0	0	0
			61	42	2	7	10			
2	H	6	Total	C	Cl	N	O	0	0	0
			61	42	2	7	10			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

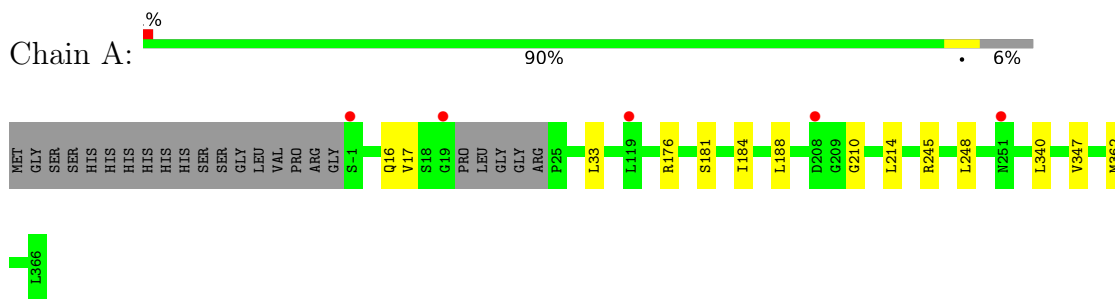
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total 129	O 129	0	1
5	B	98	Total 98	O 98	0	0
5	C	96	Total 96	O 96	0	0
5	D	95	Total 95	O 95	0	0



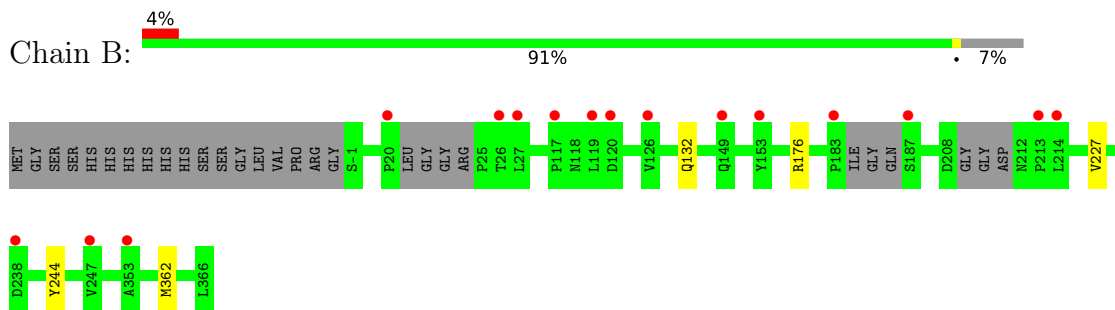
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

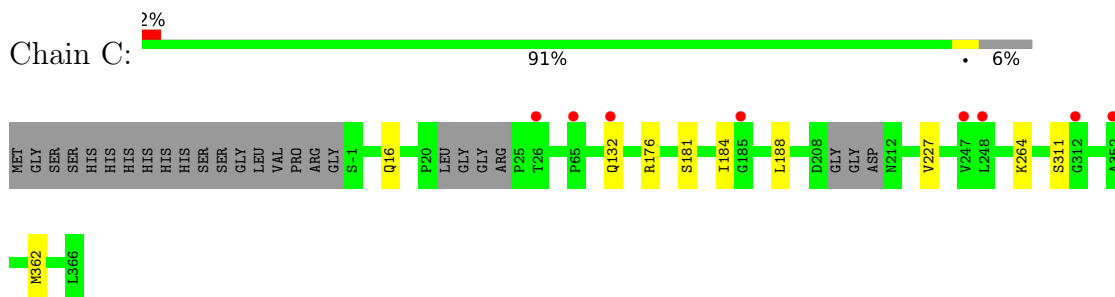
- Molecule 1: Beta sliding clamp



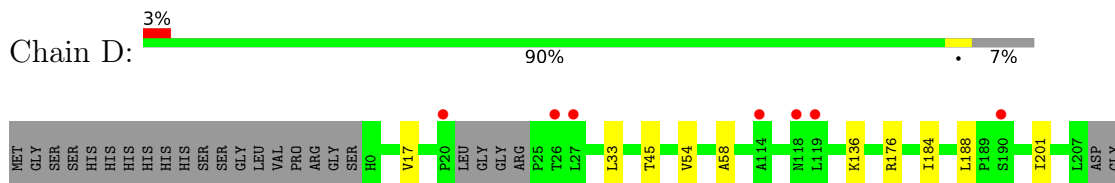
- Molecule 1: Beta sliding clamp

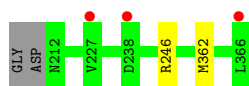


- Molecule 1: Beta sliding clamp



- Molecule 1: Beta sliding clamp





- Molecule 2: Peptide 38

Chain E: 83% 17%



- Molecule 2: Peptide 38

Chain G: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: Peptide 38

Chain F: 83% 17%



- Molecule 2: Peptide 38

Chain H: 100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.61Å 86.64Å 153.90Å 90.00° 92.56° 90.00°	Depositor
Resolution (Å)	70.69 – 2.42 153.74 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.69-2.42) 87.6 (153.74-2.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.43Å)	Xtrriage
Refinement program	BUSTER	Depositor
R, $R_{free}$	0.208 , 0.233 0.213 , 0.243	Depositor DCC
$R_{free}$ test set	3558 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.2	Xtrriage
Anisotropy	0.647	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	0.105 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZCL, SJW, SOQ, PEG, GOL, ALC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	0/2858	0.59	0/3871
1	B	0.37	0/2825	0.59	0/3823
1	C	0.36	0/2852	0.59	1/3862 (0.0%)
1	D	0.37	0/2821	0.59	0/3819
2	E	0.19	0/15	0.46	0/17
2	F	0.42	0/15	0.63	0/17
2	G	0.53	0/15	0.52	0/17
2	H	0.40	0/15	0.51	0/17
All	All	0.37	0/11416	0.59	1/15443 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	LYS	CG-CD-CE	6.28	130.75	111.90

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2808	0	2793	4	0
1	B	2778	0	2771	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2798	0	2792	2	0
1	D	2773	0	2781	5	0
2	E	61	0	39	1	0
2	F	61	0	39	0	0
2	G	70	0	38	0	0
2	H	61	0	39	0	0
3	A	6	0	8	0	0
4	B	7	0	10	0	0
4	D	7	0	10	1	0
5	A	129	0	0	0	0
5	B	98	0	0	0	0
5	C	96	0	0	0	0
5	D	95	0	0	1	0
All	All	11848	0	11320	13	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 13 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ILE:HD11	1:D:188:LEU:HD21	1.93	0.51
1:A:184:ILE:HD11	1:A:188:LEU:HD21	1.93	0.50
1:C:184:ILE:HD11	1:C:188:LEU:HD21	1.93	0.48
1:D:136:LYS:HA	5:D:563:HOH:O	2.14	0.47
1:A:340:LEU:HD23	1:A:347:VAL:CG1	2.47	0.45

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	360/386 (93%)	352 (98%)	7 (2%)	1 (0%)	41	54
1	B	350/386 (91%)	341 (97%)	9 (3%)	0	100	100
1	C	357/386 (92%)	348 (98%)	9 (2%)	0	100	100
1	D	353/386 (92%)	345 (98%)	8 (2%)	0	100	100
2	E	2/6 (33%)	2 (100%)	0	0	100	100
2	F	2/6 (33%)	2 (100%)	0	0	100	100
2	G	2/6 (33%)	2 (100%)	0	0	100	100
2	H	2/6 (33%)	2 (100%)	0	0	100	100
All	All	1428/1568 (91%)	1394 (98%)	33 (2%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/330 (93%)	303 (98%)	5 (2%)	62	78
1	B	305/330 (92%)	302 (99%)	3 (1%)	76	87
1	C	306/330 (93%)	301 (98%)	5 (2%)	62	78
1	D	303/330 (92%)	299 (99%)	4 (1%)	69	83
2	E	2/2 (100%)	2 (100%)	0	100	100
2	F	2/2 (100%)	2 (100%)	0	100	100
2	G	2/2 (100%)	2 (100%)	0	100	100
2	H	2/2 (100%)	2 (100%)	0	100	100
All	All	1230/1328 (93%)	1213 (99%)	17 (1%)	67	81

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	201	ILE
1	D	362	MET
1	B	362	MET
1	C	16	GLN
1	C	176	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	GLN
1	B	217	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ALC	G	404	2	9,11,12	0.45	0	10,13,15	0.15	0
2	ALC	F	403	2	9,11,12	0.43	0	10,13,15	0.15	0
2	ALC	E	404	2	9,11,12	0.42	0	10,13,15	0.19	0
2	ZCL	H	407	2	13,14,14	0.15	0	18,19,19	0.26	0
2	ALC	H	404	2	9,11,12	0.39	0	10,13,15	0.19	0
2	ZCL	F	406	2	13,14,14	1.13	2 (15%)	18,19,19	1.17	2 (11%)
2	ZCL	G	407	2	13,14,14	0.16	0	18,19,19	0.48	0
2	ZCL	E	407	2	13,14,14	0.11	0	18,19,19	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALC	G	404	2	-	0/5/14/16	0/1/1/1
2	ALC	F	403	2	-	0/5/14/16	0/1/1/1
2	ALC	E	404	2	-	0/5/14/16	0/1/1/1
2	ZCL	H	407	2	-	2/8/8/8	0/1/1/1
2	ALC	H	404	2	-	1/5/14/16	0/1/1/1
2	ZCL	F	406	2	-	2/8/8/8	0/1/1/1
2	ZCL	G	407	2	-	2/8/8/8	0/1/1/1
2	ZCL	E	407	2	-	2/8/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	406	ZCL	O-C	2.94	1.31	1.22
2	F	406	ZCL	OXT-C	-2.60	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	406	ZCL	OXT-C-CA	3.54	125.43	113.38
2	F	406	ZCL	O-C-CA	-3.29	110.53	122.14

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	404	ALC	O-C-CA-CB
2	F	406	ZCL	N-CA-CB-CG
2	H	407	ZCL	N-CA-CB-CG
2	H	407	ZCL	C-CA-CB-CG
2	E	407	ZCL	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PEG	D	401	-	6,6,6	0.18	0	5,5,5	0.17	0
3	GOL	A	401	-	5,5,5	0.23	0	5,5,5	0.26	0
4	PEG	B	401	-	6,6,6	0.09	0	5,5,5	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	D	401	-	-	1/4/4/4	-
3	GOL	A	401	-	-	4/4/4/4	-
4	PEG	B	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	PEG	O2-C3-C4-O4
3	A	401	GOL	O1-C1-C2-C3
3	A	401	GOL	C1-C2-C3-O3
3	A	401	GOL	O1-C1-C2-O2
3	A	401	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	PEG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	363/386 (94%)	-0.02	5 (1%) 75 73	18, 37, 66, 92	0
1	B	358/386 (92%)	0.24	16 (4%) 33 31	29, 49, 83, 106	0
1	C	361/386 (93%)	0.21	8 (2%) 62 59	28, 50, 78, 103	0
1	D	359/386 (93%)	0.18	10 (2%) 53 50	26, 49, 80, 105	0
2	E	2/6 (33%)	0.20	0 100 100	38, 38, 38, 39	0
2	F	2/6 (33%)	0.11	0 100 100	36, 36, 36, 49	0
2	G	2/6 (33%)	-0.16	0 100 100	33, 33, 33, 46	0
2	H	2/6 (33%)	0.10	0 100 100	36, 36, 36, 40	0
All	All	1449/1568 (92%)	0.15	39 (2%) 54 52	18, 46, 78, 106	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	366	LEU	5.5
1	B	20	PRO	5.2
1	D	26	THR	4.3
1	B	119	LEU	4.0
1	C	185	GLY	3.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZCL	F	406	14/14	0.76	0.23	56,73,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZCL	E	407	14/14	0.82	0.29	70,87,100,101	0
2	ZCL	G	407	14/14	0.84	0.20	47,74,82,98	0
2	ZCL	H	407	14/14	0.86	0.18	33,67,75,82	0
2	ALC	F	403	11/12	0.89	0.19	38,42,54,55	0
2	ALC	H	404	11/12	0.91	0.15	36,42,49,62	0
2	ALC	E	404	11/12	0.93	0.18	32,37,44,50	0
2	ALC	G	404	11/12	0.96	0.15	36,49,52,66	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PEG	D	401	7/7	0.87	0.18	46,51,54,59	0
3	GOL	A	401	6/6	0.92	0.19	35,40,41,46	0
4	PEG	B	401	7/7	0.93	0.12	32,37,46,47	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.